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Model study of interplay of superconductivity and magnetism in cuprate superconductors

B Pradhan[1]*, G C Rout[2] and S N Behera[3]†

[1]Department of Physics, Government Science College, Nuapada-766 105, Orissa, India
[2]Condensed Matter Physics Group, Government Science College, Chatrapur-761 020, Orissa, India
[3]Institute of Physics, Sachivalaya Marg, Bhubaneswar-751 005, Orissa, India

E-mail : brunda@iopb.res in

Abstract : The compitition between magnetism and superconductivity is investigated in cuprate superconductors of type $R_{1-x}M_xCuO_4$ [R = La, Nd; M = Sr, Ba, Ce]. The anti-ferromagnetic long range ordering and the superconducting ordering are associated with the same conduction electrons and hence there is strong interplay between the two phenomena A model is proposed for the interplay of the two types of orderings. Zubarev's double time Green's function technique and equations of motion method is used to evaluate the superconducting gap and anti-ferromagnetic staggered field. The interplay is studied by varying the coupling parameters, the position of the *f*-level and the hybridisation. The results are discussed.

Keywords : Anti-ferromagnetic order, magnetic superconductors, Cu-O plane.

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1. Introduction

Doping of charge carriers into the Mott-type anti-ferromagnet of nondoped high-T_c cuprates induces remarkable changes in the magnetic as well as transport properties. The doping transforms the insulating anti-ferromagnetic (AFM) in to the normal or conventional metallic one with increasing the doping rate; the high-T_c superconducting (SC) phase appears in between the two. Although the mechanism of the pairing interaction of high-T_c superconductivity is not fully understood at present, the interplay between the magnetic fluctuations and high-T_c superconductivity is one of the central issues in the basic physics of the Lamellar CuO_2 materials. The phase diagram of the hole doped $La_{2-x}Sr_xCuO_4$ (named LSCO) and electron doped $Nd_{2-x}Ce_xCuO_4$ (named NCCO) illustrate the ground state behaviour of the superconducting state. The holes introduced into LSCO destroy the 3-d long range Néel order with x ~0.02 [1]. In between x ~0.02 and x ~0.05, a so called spin-glass phase appears. Superconducting phase develops with *Sr* doping beyond x ~0.05. At the same time, incommensurate spatial spin modulation appears with magnetic inelastic scattering peaks on the 2-d reciprocal planer [2], T_c reaches a maximum of about 38 K around optimal doping, t ~0.15 [3]. In between x ~0.05 to 0.15, there exists an anomalous doping near x = 1/8, where the superconductivity is locally suppressed down to ~25 K. Over doping beyond x ~0.15 degrades the superconductivity and beyond x ~0.27, the superconductivity disappears. The pairing mechanism of the high-T_c materials is not yet clear. Based on these studies, one concludes that the superconducting phase may be accompanied by the antiferromagnetic spin density wave states. In this present communication, we attempt to study the inter play of superconductivity and anti-ferromagnetism in high-T_c cuprates through a microscopic model.

2. Theoretical model

The anti-ferromagnetism (AFM) is due to the same itinerant electron which are responsible for superconductivity (SC). Then the former is more likely to be of the form of a spin-density-wave (SDW) arising

*Corresponding Author
†Present Address : Berhampur University, Bhanja Vihar, Berhampur-760 007, Ganjam, Orissa, India

from a Fermi surface instability. A mean field description of the coexistence of SDW and SC with different order parameters has been studied recently [1]. In the present model, the AFM arises due to sub-lattice magnetization arising from the conduction electrons which are again responsible for SC. In addition, the localized f-electrons of the rare-earth atoms and the itinerant conduction electrons hybridize. Fulde *et al* [5] have earlier proposed such a model to describe the heavy fermion behaviour observed in copper oxide superconductors. Rout *et al* and coworkers have applied this model in presence of electron-phonon interaction with the hybridization between the f-level and the itinerant electrons states to describe Raman spectra of the high-T_c cuprates in normal state. The coexistence of the SC and AFM in cuprates and in borocarbide superconductors is studied within the Fulde model in presence of a BCS type s-wave Cooper pairing in absence of f-level [7,8]. Recently, we have reported the theoretical studies of the SC gap of the non-magnetic superconducting state of cuprate system in presence of f-level [8]. Here we present the co-existent phase of cuprate systems in presence of the f-level position of rare-earth atom. The model Hamiltonian is given below.

$$H = H_c + H_s + H_f + H_v + H_1. \tag{1}$$

H_c describes the hopping of the conduction electrons between the neighbouring sites of the two sub-lattices and is given by

$$H_c = \sum_{k,\sigma} \epsilon_0(k)\left(a^{\dagger}_{k,\sigma} b_{k,\sigma} + H.C.\right). \tag{2}$$

Here, $a^{\dagger}_{k,\sigma}$ ($a_{k,\sigma}$) and $b^{\dagger}_{k,\sigma}$ ($b_{k,\sigma}$) are creation (annihilation) operators of the conduction electrons of copper ions at two sub-lattices 1 and 2 respectively with momentum k and spin σ. The hopping takes place between neighbouring sites of copper with dispersion $\epsilon_0(k) = -2t_0(\cos k_x + \cos k_y)$. The sub-lattice magnetization arises from the Heisenberg exchange interaction between the magnetic moments at the neighbouring sites. The Hamiltonian for the staggered sub-lattice magnetisation can be written within mean field approximation as

$$H_c = \frac{h}{2}\sum_{k,\sigma} \sigma\left(a^{\dagger}_{k,\sigma} a_{k,\sigma} - b^{\dagger}_{k,\sigma} b_{k,\sigma}\right), \tag{3}$$

where h *is* the strength of sub-lattice magnetisation (=AFM order parameter) due to the conduction electron and is defined as

$$h = -\frac{h}{2} g_L \mu_B \sum_{k,\sigma}\left[\left\langle a^{\dagger}_{k,\sigma} a_{k,\sigma}\right\rangle - \left\langle b^{\dagger}_{k,\sigma} b_{k,\sigma}\right\rangle\right] \tag{4}$$

g_L and μ_B being the Lande-g factor and Bohr magneton respectively. The intra f-electron Hamiltonian H_f is described by

$$H_f = \epsilon_f \sum_{k,\sigma}\left(f^{\dagger}_{1,k,\sigma} f_{1,k,\sigma} - f^{\dagger}_{2,k,\sigma} f_{2,k,\sigma}\right), \tag{5}$$

where ϵ_f *is* the dispersionless renormalized f-level energy of the rare-earth ion and $f^{\dagger}_{i,k,\sigma}$ ($f_{i,k,\sigma}$) is the creation (annihilation) operator of the localized electron in the sub-lattice i = 1, 2. There exists a weak hybridization between the 3d conduction electrons of copper and f-electrons of the rare-earth atom with a momentum independent hybridization strength V. The Hamiltonian describing this hybridization is given by

$$H_v = V\sum_{k,\sigma}\left(a^{\dagger}_{k,\sigma} f_{1,k,\sigma} + b^{\dagger}_{k,\sigma} f_{2,k,\sigma} + H.C.\right). \tag{6}$$

Finally, the mean field BCS Hamiltonian describing phonon mediated superconductivity at the two different sites of copper (assuming only intra sub-lattice pairing)

$$H_l = -\Delta \sum_k \left[\left(a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} + H.C.\right)\right. \tag{7}$$

$$\left. + \left(b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow} + H.C.\right)\right].$$

The inter sub-lattice pairing though significant, is not taken into consideration for simplicity of numerical calculations. Here Δ is the superconducting gap parameter given by

$$\Delta = -\sum \bar{V}_K \left[\left\langle a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow}\right\rangle + \left\langle b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow}\right\rangle\right], \tag{8}$$

$\bar{V}_k$ being the strength of the attractive interaction between two electrons mediated by the phonons or other medium. It is to be noted that the total Hamiltonian of the system is a mean field one which can be solved exactly. We have used the equations of motion method for calculation of the single particle Green's functions by Zubarev's technique [10].

3. Calculation of AFM and SC order parameters

We can calculate one electron Green's functions using the Hamiltonian given in eq. (1) for the superconducting state of the cuprate systems. Out of the eight first site Green's functions $A_i(k,\omega)$ (i = 1–8) involved in these calculations, the first two Green's functions are defined

$$A_1(k,\omega) = \langle\langle a_{k\uparrow}; a^\dagger_{k\uparrow}\rangle\rangle,$$

$$A_2(k,\omega) = \langle\langle a^\dagger_{-k\downarrow}; a^\dagger_k \qquad (9)$$

The coupled equations are solved exactly to find out the two required Green's functions *i.e*, $A_{1,2}(k,\omega)$ as

$$A_1 = \frac{1}{2\pi|D_{12}|}\left[|D_0||D_3| - \epsilon_0^2\left(\omega^2-\epsilon_f^2\right)|D_4|\right], \qquad (10)$$

$$= \frac{-\Delta\left(\omega^2-\epsilon_f^2\right)}{2\pi|D_{12}|}\left[|D_0| - \epsilon_0^2\left(\omega^2-\epsilon_f^2\right)|D_4|\right], \qquad (11)$$

where

$$|D_{12}| = |D_1||D_2| - 4\epsilon_f^2\epsilon_k^2\, v^4, \qquad (12)$$

$$|D_1|, |D_2| = \left[\left(\omega^2 - E^2_{1,2k}\right)\left(\omega^2-\epsilon_f^2\right) - 2\omega^2 v^2 + v^4\right], \qquad (13)$$

$$E^2_{1,2}(k) = \epsilon_0^2(k) + (h/2 \mp \Delta)^2, \qquad (14)$$

$$\epsilon_k^2 = \epsilon_0^2 + h^2/4, \qquad (15)$$

(8) $$|D_0| = \left\{(\omega+h/2)^2 - \Delta^2\right\}(\omega^2-\epsilon_f^2) \qquad (16)$$

$$-2(\omega+h/2)\omega v^2 + v^4,$$

$$|D_3|, |D_4| = (\omega \mp h/2)(\omega^2-\epsilon_f^2)(\omega - \epsilon_f)v^2. \qquad (17)$$

Similarly out of the eight second site Green's functions $B_i(k,\omega)$(i = 1–8) involved in the calculations, the first two Green's functions are defined as

$$B_1(k,\omega) = \langle\langle b_{k\uparrow}; b^\dagger_{k\uparrow}\rangle\rangle_\omega,$$

$$B_2(k,\omega) = \langle\langle b^\dagger_{-k\downarrow}; b^\dagger_{k\uparrow}\rangle\rangle_\omega. \qquad (18)$$

The coupled equations are solved exactly to find out the Green's functions *i.e*, $B_{1,2}(k,\omega)$ as

$$B_1 = \frac{1}{2\pi|D_{12}|}\left[|D_0'||D_4| - \epsilon_0^2\left(\omega^2-\epsilon_f^2\right)|D_3|\right], \qquad (19)$$

$$B_2 = \frac{-\Delta\left(\omega^2-\epsilon_f^2\right)}{2\pi|D_{12}|}\left[|D_0'| - \epsilon_0^2\left(\omega^2-\epsilon_f^2\right)\right], \qquad (20)$$

where

$$|D_0'| = \left\{(\omega-h/2)^2 - \Delta^2\right\}(\omega^2-\epsilon_f^2) \qquad (21)$$

$$-2\omega v^2(\omega-h/2) + v^2.$$

The poles of the Green's functions $A_2(k,\omega)$ and $B_2(k,\omega)$ give eight quasi-particle energy bands. However, it is difficult to calculate the quasi-particle band from $|D_{12}|$ in eq. (12) which is a polynomial of the order eight. We simplify the problem by assuming that the f-electron level (ϵ_f) is close to the Fermi level and the hybridization is weak. Hence we neglect ϵ_f^2 and v^4 from $|D_{12}|$ given in eq. (12). The condition $|D_{12}| \simeq |D_1||D_2| = 0$ gives eight quasi-particle energy bands $\pm\omega_i$ (i = 1–4) as given below

$$\pm\omega_{1,2} = \left[\frac{S_1 \pm \sqrt{S_1^2 - 4T_1}}{}\right]^{1/2}$$

$$\pm\omega_{3,4} = \left[\quad\right]^{1/2} \qquad (22)$$

where

$$S_1 = E_{1k}^2 + \epsilon_f^2 + 2v^2,$$

$$T_1 = E_{1k}^2\,\epsilon_f^2 + v^2,$$

$$S_2 = E_{2k}^2 + \epsilon_f^2 + 2\upsilon^2,$$

$$T_2 = E_{2k}^2 \epsilon_f^2 + \upsilon^2. \qquad (23)$$

The SC parameters defined in eq. (8) is calculated from the Green's functions $A_2(k,\omega)$ and $B_2(k,\omega)$ given in eqs. (11) and (20).

$$\Delta = -\frac{1}{2} g \int_{-\omega D}^{\omega D} \Delta d \epsilon_0 \left[H_1(T) - H_2(T) \right], \qquad (24)$$

where

$$H_1(T) = \frac{1}{\omega_1^2 - \omega_2^2} (F_1(T) - F_2(T)), \qquad (25)$$

$$H_2(T) = \frac{1}{\omega_3^2 - \omega_4^2} (F_3(T) - F_4(T)), \qquad (26)$$

$$F_\alpha(T) = \frac{1}{\omega_\alpha h \Delta} \left(\omega_\alpha^2 - \epsilon_0^2 - \Delta^2 + h^2/4 \right)$$

$$\left(\omega_\alpha^2 - \epsilon_f^2 \right) - 2\omega_\alpha^2 \upsilon^2 + \upsilon^4 \left(\tanh \frac{\beta \omega_\alpha}{2} \right), \qquad (27)$$

where $\alpha = 1$ to 4. The AFM parameter defined in eq. (4) is calculated from the Green's functions $A_1(k,\omega)$ and $B_1(k,\omega)$ given in eqns. (10) and (19).

$$h = -\frac{1}{4} g_1 \int_{-WD}^{+WD} h d \epsilon_0 \left[H_3(T) - H_4(T) \right], \qquad (28)$$

where

$$H_3(T) = \frac{1}{\omega_1^2 - \omega_2^2} (G_1(T) - G_2(T)), \qquad (29)$$

$$H_4(T) = \frac{1}{\omega_3^2 - \omega_4^2} (G_3(T) - G_4(T)), \qquad (30)$$

$$G_2(T) = \frac{P_\alpha(\omega_\alpha) f_\alpha(\omega_\alpha) - Q_\alpha(-\omega_\alpha) f_\alpha(-\omega_\alpha)}{\omega_\alpha h \Delta}, \qquad (31)$$

$$P_\alpha(\omega_\alpha) = \left(\omega_\alpha^2 - \epsilon_f^2 \right)^2 \left(\omega_\alpha^2 - h^2/4 + \Delta^2 - \epsilon_0^2 \right)$$

$$-\upsilon^2 \left(\omega_\alpha - \epsilon_f \right)^2 \left(2\omega_\alpha^2 - 2\omega_\alpha \epsilon_f + f^2 \right), \qquad (32)$$

$$Q_\alpha(-\omega_\alpha) = \left(\omega_\alpha^2 - \epsilon_f^2 \right)^2 \left(\omega_\alpha^2 - h^2/4 + \Delta^2 - \epsilon_0^2 \right)$$

$$-\upsilon^2 \left(\omega_\alpha - \epsilon_f \right)^2 \left(2\omega_\alpha^2 - 2\omega_\alpha \epsilon_f + \upsilon^2 \right) \qquad (33)$$

and the Fermi functions are

$$f(\pm\omega_\alpha) = \left[1 + \exp(\beta \pm \omega_\alpha)^{-1} \right].$$

$N(0)$ is the density of states of conduction electrons at the Fermi level. The different physical quantities of the atomic sub-system are made dimensionless dividing them by the hopping integral $2t_0$. The width of the conduction band is $W = 8t_0$. The dimensionless parameters are given by

$$z = \frac{\Delta}{2t_0},\ g = N(0)V_0,\ \tilde{\omega}_D = \frac{\omega_D}{2t_0},\ t = \frac{K_B T}{2t_0}$$

$$h1 = \frac{h}{2t_0},\ g1 = N(0) g_L \upsilon_B,\ d = \frac{\epsilon_f}{2t_0},\ \upsilon = \frac{v}{2t_0}$$

4. Results and discussion

It is seen from the gap equations (24) and (28), that the SC gap z and the AFM gap h_1 are the functions of themselves and the chemical potentials. So the gap equations are solved self-consistently under the half filling band situations with the Fermi level lying at the middle of the conduction band. The different reduced parameters involved in the numerical calculations are the SC gap z, the AFM gap h_1, f-level position d, the hybridization strength υ and the reduced temperature t. Here, we have taken the conduction band width $W = 8t_0 \simeq 1$ eV and the Debye frequency $\omega_D \simeq 250$ K for the high-T_c superconductors. The interplay of the SC gap z and the AFM leads to two situations *i.e*, $T_N > T_c$ and $T_N < T_c$ for both the borocarbide as well as high-T_c superconductors. We report below only the former situation and discuss the effect of the interplay and parameter dependence of both the gaps for systems like $R_{2-x}Ce_xCuO_4$ (R = Gd, Tm,....).

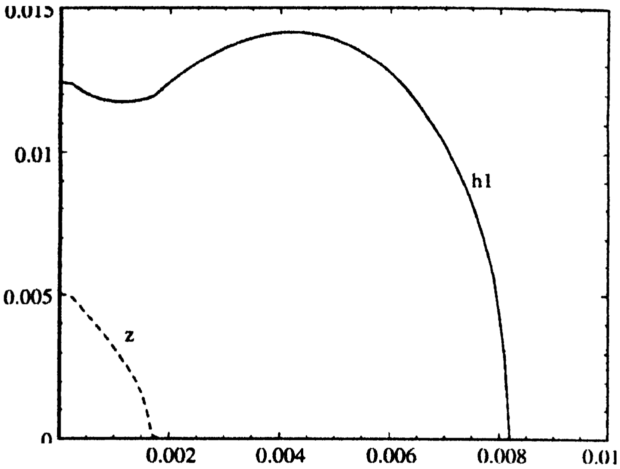

Figure 1. The self-consistent plot of z, hl *vs* t for fixed values of d = 0.00089, v = 0.0003, g = 0.190 and gl = 0.110.

For the choice of the SC coupling g = 0.190 and the AFM coupling g_1 = 0.110, the temperature dependence of the SC gap z and the AFM gap $h1$ in the coexistence phase of the system is depicted in Figure 1. This choice of g and $g1$ describes the system for the Néel temperature t_N is greater than the SC transition temperature T_c. The temperature dependence of the SC gap z exhibits mean field behaviour with $z(t = 0) \simeq 0.005$ and $t_c \simeq 0.0015$ giving a value of $2\Delta(0)/K_BT_c \simeq 5.0$ which is greater than the BCS universal value of 3.52. This high value is compatible with the results of the high-T_c superconductors. On the other hand, the AFM gap $h1$ also exhibits mean field behaviour with a depression of the gap at low temperatures. On lowering the temperature for $t < t_N$, the AFM gap parameter increases to a broad maximum at $\frac{t_N}{2}$ and then decreases towards low temperatures with a minima at a temperature t_m, then increases towards low temperature. In the temperature range $t_c < t < t_N/2$, the decrease in AFM gap is due to the paramagnetic spin fluctuation above the SC transition temperature and the minima occurs where the SC phase develops. The depression in AFM gap at low temperature is due to the onset of the superconductivity and the spin nipping during the coexistence phase due to the hybridization between the conduction electron and the f-electrons. Also this depression in AFM gap in coexistence phase might be enhanced due to the proximity of the f-level of the rare-earth atom. The anomalous behaviour of the AFM gap at low temperatures may be explained due to the formation of AFM order in the f-electron. Further the formation of the SC pairing amplitudes of the type : mixed pairing $\phi^{af} = \langle a^{\dagger}_{k\uparrow} f^{\dagger}_{-k\downarrow}\rangle$, $\phi^{bf} = \langle b^{\dagger}_{k\uparrow} f^{\dagger}_{-k\downarrow}\rangle$ and f-level pairing $\phi^{f} = \langle f^{\dagger}_{k\uparrow} f^{\dagger}_{-k\downarrow}\rangle$, may be responsible for the depression of the AFM gap at low temperatures. The effect of the SC coupling g on SC gap and the AFM gap are illustrated in Figures 2 and 3 and the effects of the AFM coupling $g1$ on the SC gap and the AFM gap are shown in Figures 4 and 5.

Figure 2 shows the self-consistent plot of z *vs* t in the coexistence phase of the system. It is observed that the increase in the SC coupling g leads to the suppression

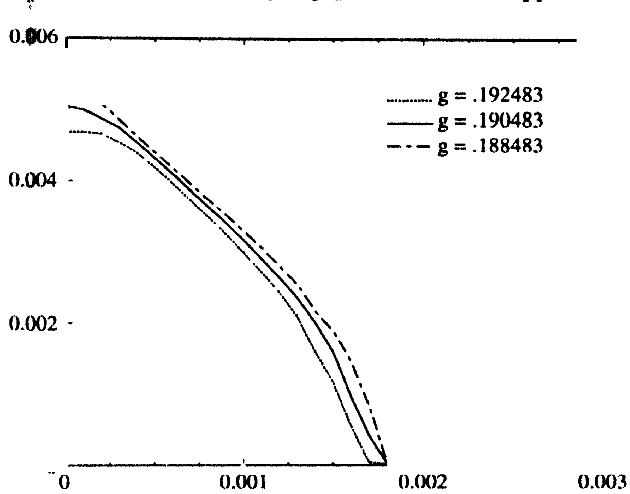

Figure 2. The self-consistent plot of z *vs* t for fixed values of d = 0.00089, v = 0.0003 and gl = 0.110 and different values of g = 0.192, 0.190 and 0.188.

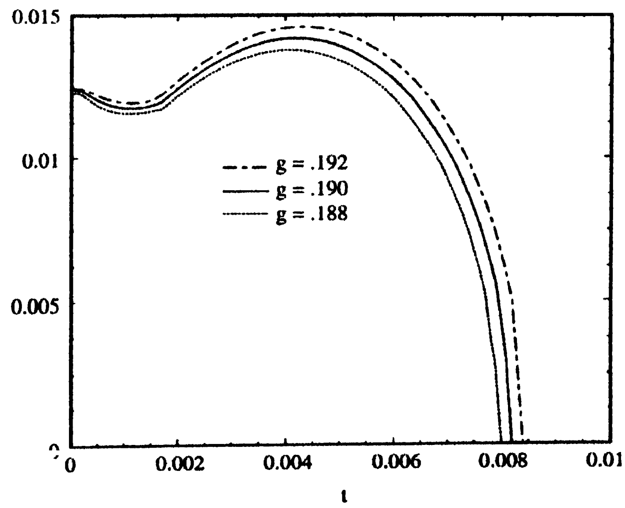

Figure 3. The self-consistent plot of hl *vs* t for fixed values of d = 0.00089, v = 0.0003 and gl = 0.110 and different values of g = 0.192, 0.190 and 0.188.

of the SC gap throughout the temperature range, besides the suppression of the SC transition temperature. This type of behaviour is also observed in a model study of the superconductivity and spin-density-wave (SDW) state [11]. The effect of the SC coupling on the AFM gap is shown in Figure 3. The increase of the SC coupling increases the AFM gap throughout the temperature range accompanied by the enhancement of the Neel temperature. Thus it appears that the SC coupling g acts as the AFM coupling.

Figure 4 illustrates the variation of the SC gap due to the change of the AFM coupling. The increase of AFM coupling enhances the SC gap z throughout the temperature range besides enhancing the SC transition temperature. Thus it appears the presence of the AFM order helps in enhancing the SC order. Figure 5 shows

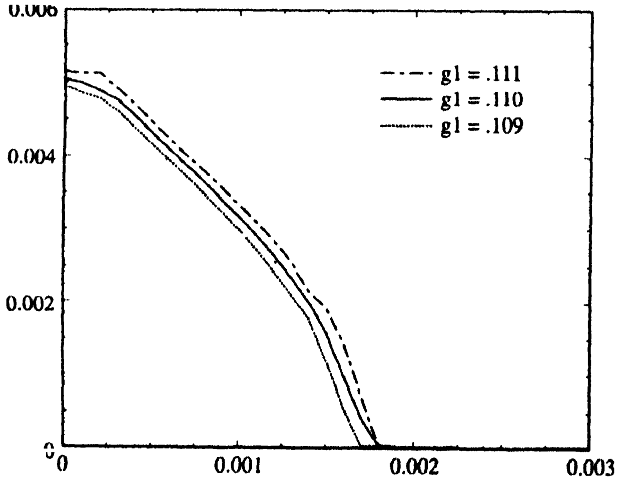

Figure 4. The self-consistent plot of z *vs* t for fixed values of d = 0.00089, υ = 0.0003 and g = 0.190 and different values of gl = 0.111, 0.110 and 0.109.

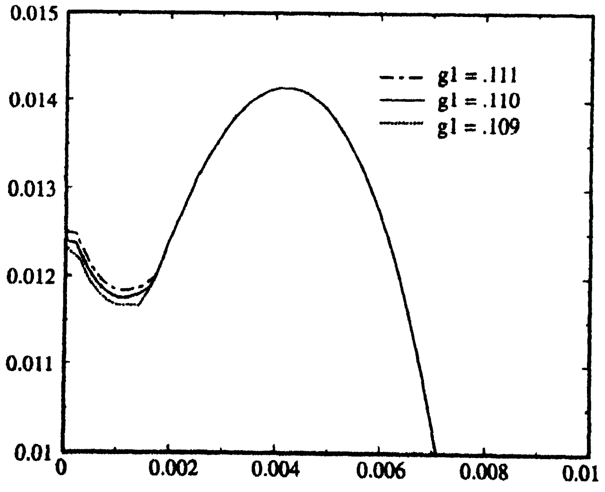

Figure 5. The self-consistent plot of hl *vs* t for fixed values of d = 0.00089, υ = 0.0003 and g = 0.190 and different values of gl = 0.111, 0.110 and 0.109.

the effect of AFM coupling on the AFM gap. The AFM coupling has no effect on the AFM and Néel temperature in the normal magnetic phase in the temperature range $t_c < t < t_N$. However the AFM coupling gl enhances the AFM gap in the coexistence of the SC-AFM phase in the temperature $t < t_c$. Thus it appears the AFM long range order and the SC order enhance each other in the co-existence phase. This type of behaviour is observed in the SC-SDW co-existence phase in high-T_c phase [11] and also in high-T_c systems [7,8].

5. Conclusion

We have formulated a model for high-T_c cuprates describing the co-existence of AFM order and SC order due to the conduction electrons in presence of the hybridization between the conduction electrons and the f-electrons of the rare-earth atom, with f-electron energy level lying above the Fermi level. A part of the co-existence phase results is reported in this communication with an emphasis on the position of the f-level of the rare-earth atom which acts as an impurity in the *Cu–O* plane in the electron doped cuprate systems. The co-existence of the AFM and the SC phase at low temperatures gives rise to a depression in the AFM gap which may be due to the spin flipping, due to the formation of either the SC pairing in conduction electrons or the f-electrons. It appears as if the SC coupling acts as the AFM coupling resulting in enhancement for the AFM gap as well as Néel temperature. However the AFM coupling enhances both the SC order and the AFM order in the co-existence phase at low temperatures. Hence the co-existence phase is conducive to both the AFM long range order and the SC order in these systems.

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